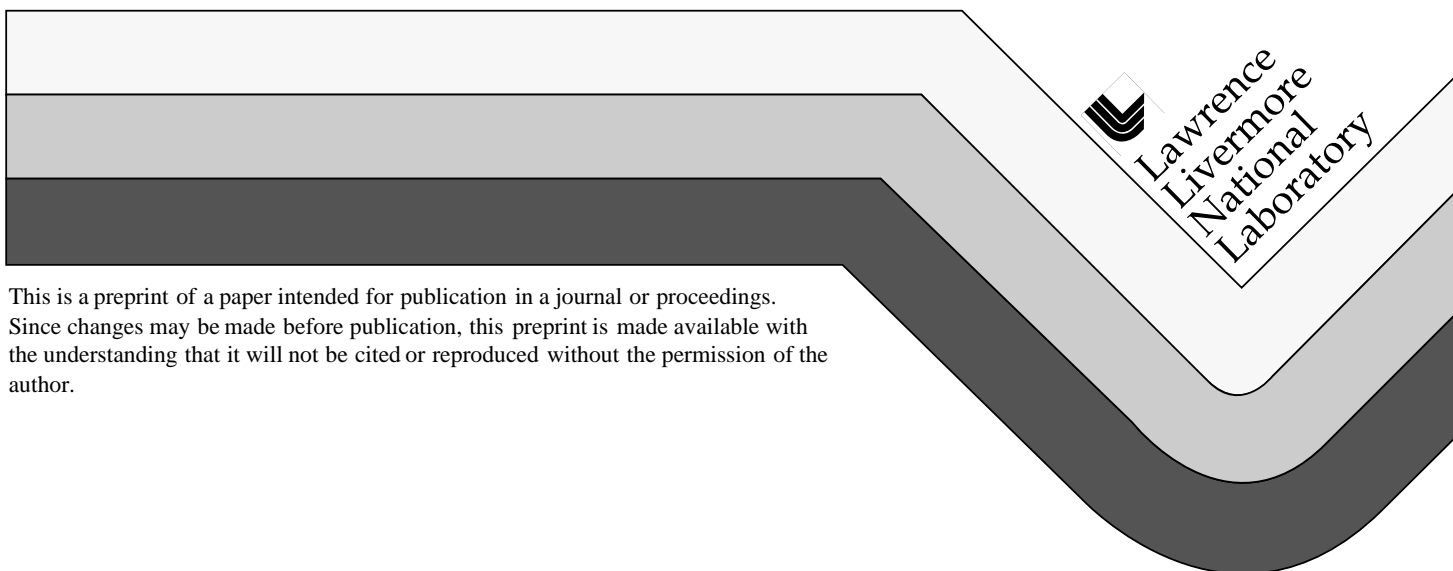


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A New Computational Method for non-LTE, the Linear Response Matrix

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We investigate non-local thermodynamic equilibrium atomic kinetics using nonequilibrium thermodynamics and linear response theory. This approach gives a rigorous general framework for exploiting results from non-LTE kinetic calculations and offers a practical data-tabulation scheme suitable for use in plasma simulation codes. We describe how this method has been implemented to supply a fast and accurate non-LTE option in Lasnex.

Keywords: opacity, non-local thermodynamic equilibrium, non-LTE, NLTE, linear response matrix

Introduction

Extensive theoretical and computational calculations have been done that lay the ground work for a linear response matrix method to calculate non-LTE (non-local thermodynamic equilibrium) opacities. We will briefly review some of this work and describe what has been done to utilize this theory to create a computational package to rapidly calculate mild non-LTE emission and absorption opacities suitable for use in hydrodynamic calculations. The opacities are obtained by performing table look-ups on data that has been generated off-line with a non-LTE package. This scheme is currently under development. We can see that it offers a significant computational speed advantage over non-LTE calculations performed in-line. It is suitable for mild non-LTE, quasi-steady conditions. And it offers a new insertion path for high-quality non-LTE data. Currently, the linear response matrix data file is created using XSN¹, but these files could be generated by more detailed and rigorous calculations without changing any part of the implementation in the hydro code. The scheme is running in Lasnex and is being tested and developed.

(Brief) Review of Previous Work on the Linear Response Matrix

The radiative properties of dense plasmas, such as stellar interiors, are usually studied using LTE methods. But we are often interested in applications that require non-equilibrium kinetic

1. W.A. Lokke and W. Grasberger, UCRL-52276 (1977); G. B. Zimmerman and R. M. More, J. Quant. Spectrosc. Radiat. Transf. **23**, 517 (1979)

models such as low density plasmas and intermediate plasmas (e.g. laser produced plasmas) that combine high densities, a significant radiation environment and non-LTE populations.

Richard More¹ and his colleagues have done extensive work to model this type of non-LTE plasma using the methods of non-equilibrium thermodynamics. They have derived a linear response matrix, $R_{\nu\nu'}$, that is *symmetric* as required by the non-equilibrium thermodynamic principles of energy conservation and minimum entropy production and by the detailed balance condition and *linear* over a surprisingly large range (even up to + or - 50% changes in the photon temperature). $R_{\nu\nu'}$ is defined as follows:

$$(\kappa_{\nu}^e - \kappa_{\nu}^a)B_{\nu} = \frac{1}{4\pi} \int R_{\nu\nu'} \left((\Delta I_{\nu'}) / \frac{\partial B_{\nu'}}{\partial T} \right) d\nu'$$

where κ_{ν}^e and κ_{ν}^a are the frequency (ν) dependent emission and absorption opacities. $\Delta I_{\nu'}$ is the perturbation of the frequency dependent photon intensity, $I_{\nu'}$, from a black body distribution, $B_{\nu'}$, (defined below) at an arbitrary frequency, ν' . T is the temperature.

Consider an ion interacting with radiation which is approximately a black body at the temperature of the free electrons. The difference between the actual radiation and the black body field causes non-equilibrium populations of excited states in the ion and leads to a net difference of emission and absorption rates. The difference of emission and absorption at frequency ν is a function of the deviation from the black body spectrum at frequency ν' and can be described as a response matrix, $R_{\nu\nu'}$.

To understand $R_{\nu\nu'}$ more fully, we will describe how it is calculated. To generate an $n \times n$ response matrix, n non-LTE calculations are performed. Each calculation is done with a photon spectrum that is perturbed by altering the black body equilibrium spectrum, $B_{\nu}(T)$, where

$$B_{\nu}(T) = A \frac{\nu^3}{\exp\left(\frac{\nu}{T}\right) - 1}$$

$B_{\nu}(T)$ is the specific intensity of radiation at frequency, ν , for a temperature, T , both in units of energy. A is a constant. The black body spectrum is perturbed by increasing the radiation intensity by a small factor, say 0.01, over a narrow frequency range centered at ν' , or this could be thought of as varying one specific line. The net radiated power at all frequencies is then calculated from the non-LTE model. It can be positive (emission) or negative (absorption) and is found to be linearly proportional to the change in the radiation intensity, $\Delta I_{\nu'} = I_{\nu'} - B_{\nu'}$, for small perturbations. When the response is linear like this, a non-LTE calculation could be replaced by a matrix multiplication of the input vector $\{I_{\nu'}\}$ representing the photon spectrum and the linear response matrix to yield the output vectors $\{\kappa_{\nu}^e\}$ and $\{\kappa_{\nu}^a\}$.

1. Richard More, p. 399 in *Atomic and Molecular Physics of Controlled Thermonuclear Fusion*, edited by C. Joachain and D. Post (Plenum, New York, 1983), S. Libby, F. Graziani, R. More and T. Kato, in *Proceedings of the International Conference on Laser Interactions and Related Plasma Phenomena*, edited by G. Miley and E. Campbell (AIP, New York, 1997)

More and Kato¹ have studied $R_{\nu\nu'}$ for aluminum at near-LTE conditions using calculations performed with the collisional-radiative (CR) model of Fujimoto and Kato² and with the Livermore XSN package which is a non-LTE, screened-hydrogenic average atom model. These two “codes” give quantitative agreement good to ~20% for the linear response matrix and it is accurately symmetric. The symmetry of the response matrix, $R_{\nu\nu'}$, does not depend on the exact model used to calculate it, the levels included in the model, the coupling scheme, atomic energy levels or cross sections. It’s exact and general and depends only on detailed balance. The symmetry of $R_{\nu\nu'}$ provides a rigorous consistency test for non-LTE models. In fact, a bug in our XSN code was found when calculations produced a non-symmetric matrix. Upon fixing the bug, XSN generated a symmetric $R_{\nu\nu'}$ matrix.

Implementation in a Simulation Code

How do we propose to use this formalism to produce fast non-LTE emission and absorption opacities for a radiation hydrodynamics code? It is the linearity of the response matrix that is the basis for the scheme. To implement it we must both create a database with a non-LTE atomic physics code and then use this database in the hydro code. Because Lasnex requires the emission and absorption opacities separately, rather than creating the linear response matrix $R_{\nu\nu'}$ described above, we form two similar $n \times n$ matrices. One is for emission opacities and one for absorption opacities. The appropriate opacities are then calculated in the code by a table look-up to account for the temperature and density dependence followed by a matrix multiply.

In our test problems, the material density, ρ , and temperature is discretized on a 13 by 15 mesh. Fifty frequency groups are used to represent the photon distribution. Fifty XSN calculations are performed to generate 50×50 matrices at each (ρ, T) point that describe the linear response of both the emission and absorption opacities at the 50 specified frequencies to perturbations at all frequencies, one by one. The LTE opacities (where the photon distribution, $I_\nu = B_\nu$) and the coronal opacities assuming $I_\nu=0$ (for future work to provide realistic limiting values) are also stored in the table at each (ρ, T) point. The required data file is then approximately $50 \times 50 \times 13 \times 15 \times 2$ long, containing about one million numbers (8 megabytes if we use double precision floating point numbers). For simplicity we choose exactly the same frequency discretization for our table and the rad-hydro calculation. In order to avoid dividing by the exponentially small numbers in the tail of the black body distribution, we divide the perturbation in the radiation distribution by dB_ν/dT , as in the definition of $R_{\nu\nu'}$.

1. Richard More and Takako Kato, PRL **81**, 814 (1998)
2. T. Fujimoto and T. Kato, Phys. Rev. **A 30**, 379 (1984)

Therefore, the values stored in the lrm (linear response matrix) table are

$$LRM_{\nu\nu'}(\rho, T) = \frac{\kappa_{\nu}^{NLTE}(\nu') - \kappa_{\nu}^{LTE}}{\left(\frac{I(\nu') - B(\nu')}{\frac{\partial}{\partial T} B(\nu')} \right)}$$

for both absorption and emission for all frequencies, ν and ν' . Also we store the LTE opacities and the coronal opacities.

Finally, the implementation in the simulation code requires reading and storing the information from the data file and using it to calculate the non-LTE opacities. To calculate the non-LTE emission and absorption opacities from the tabular data we do log-log interpolation in (ρ, T) space for each zone and frequency on the logarithm of the LTE emission and absorption opacities and on the linear response matrices, that is, on the two $n \times n$ (50 x 50) matrices. The effect of a non-LTE photon distribution on the opacity at a given frequency, ν , is then computed by a matrix multiply on the linear response matrix, by summing the linear response over all the frequencies times the corresponding perturbation of the *simulation code's* photon intensity.

$$\kappa_{\nu}(\rho, T) = \kappa_{\nu}^{LTE}(\rho, T) + \sum_{\nu'} LRM_{\nu\nu'} \left(\frac{I_{Lasnex}(\nu') - B(\nu')}{\frac{\partial}{\partial T} B(\nu')} \right)$$

We have found it necessary to impose a ceiling on the size of the perturbation, the $(I_{\nu} - B_{\nu})$ and are still testing and developing the limits of the algorithm.

Since non-LTE XSN already runs “in-line” in Lasnex, Lasnex is a perfect test bed for the new lrm algorithm. It is easy to verify that the new coding is working properly and to explore the limits of applicability of the new model, by performing the same calculation with the lrm formalism and with the full non-LTE XSN. XSN has many parameters to set. We set them carefully while generating our tables to correspond exactly to the ones that will be used in Lasnex. We have run several example calculations.

Test Calculations

The first test problem is a zero dimensional (one zone) simulation of aluminum at a low density ($\rho = .23$ g/cc) and a temperature of 100 eV in the presence of a 100 eV black body photon spectrum that has been perturbed by doubling the photon intensity for frequencies from 0.19 to 0.33 keV. See Figure 1. The lrm results compare very well with the XSN results. Figure 2. plots the relative difference between the absorption and emission opacities, $(\kappa_V^a - \kappa_V^e)/\kappa_V^a$ vs. frequency for the lrm calculation in black and for an XSN calculation with 300 groups in blue. The calculations are essentially identical, differing only because of the finer group structure in the XSN calculation. Similar simulations were performed to monitor the sensitivity of the opacities to the interpolations in (ρ, T) and the results were very reasonable.

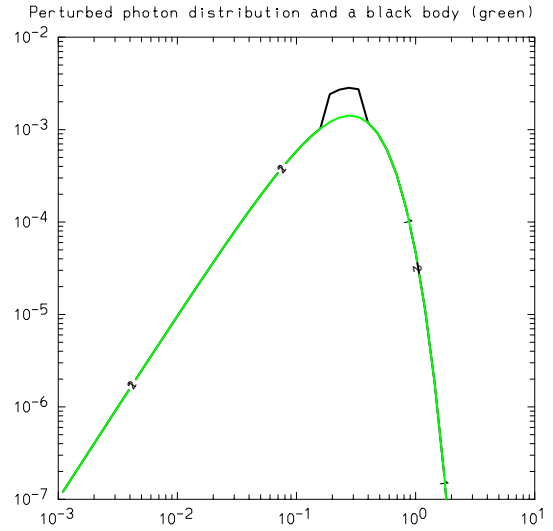


Figure 1. I_ν (jerks/cc/keV) vs. ν (keV)
Perturbed (black) and black body (green)

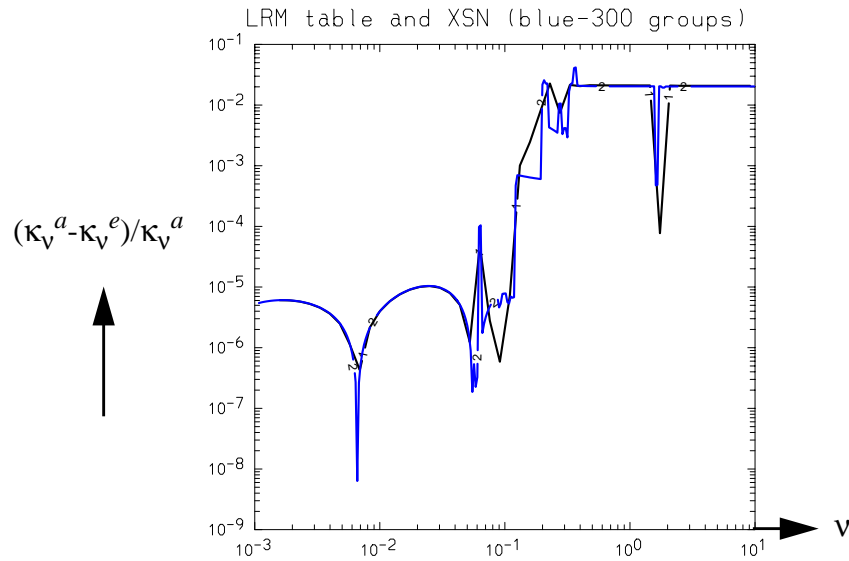


Figure 2. $(\kappa_V^a - \kappa_V^e)/\kappa_V^a$ vs. ν (keV)
lrm (black) and XSN-300 groups (blue)

A similar zero dimensional test calculations was run at a lower density ($\rho=.0016$ g/cc) and colder temperature ($T= 46$ eV) where aluminum is more in the non-LTE regime. These conditions correspond to the example used in Libby et al's paper cited earlier. The photon spectrum is perturbed as shown in Figure 3. The intensity between .19 and .33 keV was doubled. This is really quite a strong "perturbation" especially because it is near the peak of the Planckian.

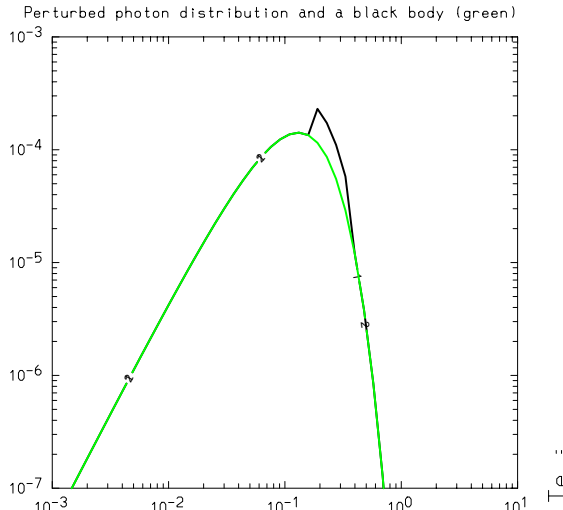


Figure 3. I_ν (jerks/cc/keV) vs. ν (keV)

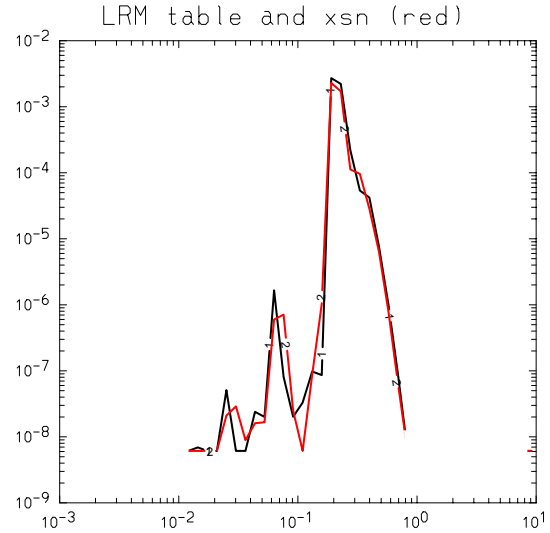


Figure 4. Emission (source function) - absorption ($\kappa_\nu^a B_\nu$) vs. ν

Using another way to display "non-LTE-ness", we plot the difference between the source function (emission opacity times the Planckian) and a similar quantity involving the absorption opacity versus frequency for the two calculations in Figure 4. We see very good agreement between the lrm (in black) and the XSN (in red) calculations. These test runs verify both the implementation of our lrm model and the linearity of the response matrix for even rather strong perturbations.

A proposed opacity experiment is to put a slab of aluminum inside a laser heated hohlraum and use a back lighter to measure the emission spectrum. The radiation environment, back light spectrum, as well as the transmission and emission spectra of the aluminum would be measured through diagnostic holes in the hohlraum. We performed simulations to model this type of experiment. A one dimensional slab of aluminum is exposed to radiation that is much hotter than the cold aluminum at say 150 keV. We found that both density and temperature profiles were essentially the same using lrm and in-line XSN. The lrm calculation took less than half the total cpu time due to a speed up of ~4 times in the opacity calculation. Larger speed-ups should be possible.

We are continuing to test and refine the linear response model in hopes that it will be a useful and efficient tool for modeling non-LTE physics, especially for the very large meshes required for three-dimensional problems.

Acknowledgements

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